Refined Second Law of Thermodynamics for Fast Random Processes

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Abstract We establish a refined version of the Second Law of Thermodynamics for Langevin stochastic processes describing mesoscopic systems driven by conservative or non-conservative forces and interacting with thermal noise. The refinement is based on the Monge-Kantorovich optimal mass transport and becomes relevant for processes far from quasi-stationary regime. General discussion is illustrated by numerical analysis of the optimal memory erasure protocol for a model for micron-size particle manipulated by optical tweezers.

Keywords Second Law of Thermodynamics · Landauer principle · Monge-Kantorovich optimal mass transport

1 Introduction

In recent years an increased interest in fluctuations of mesoscopic systems interacting with noisy environment has led to the development of "Stochastic Thermodynamics" that revisited relations between thermodynamical principles and statistical description within simple models based on stochastic differential equations, see [52, 53] and references therein. The aim of this note is to make a junction between two circles of ideas in the context of Stochastic Thermodynamics of systems whose evolution is described by the overdamped Langevin equation. One circle concerns the stochastic version [30] of the Second Law of Thermodynamics, asserting the increase of total entropy, and the related Landauer Principle [8, 38], a reformulation of the Second Law in the framework of Thermodynamics of Computation that became a subject of recent renewed interest [2, 10, 17, 18, 35, 37, 45, 56]. The other circle deals with the optimal control problems in Stochastic Thermodynamics that were recently connected in [3] to the Monge-Kantorovich optimal mass transport and the Burgers equation. The result of the junction will be a refinement, relevant for fast processes, of the Second Law of Stochastic Thermodynamics. Our improvement of the Second Law does not go in the direction of a better control of fluctuations of thermodynamical quantities [54], as do various Fluctuation Relations studied intensively in last years, see [21, 23, 33, 40]. Instead, it establishes the optimal lower bound on the total entropy production in non-equilibrium processes of fixed duration. Although the bound appeared for the first time in [3], see Eq. (19) therein, its interpretation as a refinement of the Second Law and of the Landauer principle, as well as its proof establishing its direct link to the optimal mass transport and Burgers equation rather than passing through a stochastic Bellman equation, are new. They may be viewed as a contribution to Finite-Time Thermodynamics of mesoscopic systems [1].

The paper is organized as follows. In Sect. 2, we define the concepts of performed work, heat release, and entropy production for overdamped Langevin evolution with conservative driving forces, and we recall the basic laws of Stochastic Thermodynamics. Section 3 contains a brief discussion of the relation between the Second Law of Thermodynamics and the Landauer principle. In Sect. 4, we replace the minimization of the total entropy production in overdamped Langevin processes that interpolate in a fixed time window between given statistical states by a minimization problem considered by Benamou-Brenier in [6] and shown there to be equivalent to the Monge-Kantorovich optimal mass transport problem that is the subject of Sect. 5. The latter two sections briefly review the classical mathematical results about the optimal mass transport [55] needed in our argument. In particular, the approach of [6] establishes a direct connection between the Monge-Kantorovich problem and the inviscid Burgers equation for potential velocities that plays a crucial role below. On the basis of the above results, we establish in Sect. 6 the refined version of the Second Law of Stochastic Thermodynamics. Section 7 discusses the corresponding refinement of the Landauer principle, illustrating it by the numerical analysis of a simple model of a micron-size particle in time-dependent optical traps. Section 8 extends the refined Second Law to the case of Langevin evolutions with non-conservative forces, showing that the preceding analysis covers also that case. Conclusions and remarks about open problems make up Sect. 9.

2 Stochastic Thermodynamics for Langevin Equation

We consider a small statistical-mechanical system, for example composed of mesoscopic particles, driven by time-dependent conservative forces and interacting with a noisy en-

vironment. The temporal evolution of such a system may be often well described by the overdamped stochastic Langevin equation

$$d\boldsymbol{x} = -M\nabla U(t,\boldsymbol{x})dt + d\boldsymbol{\zeta}(t) \tag{2.1}$$

in d-dimensional space of configurations with a smooth potential $U(t,\boldsymbol{x})$ and a white noise $d\boldsymbol{\zeta}(t)$ whose covariance is

$$\left\langle d\zeta^a(t) d\zeta^b(t')\right\rangle = 2D^{ab}\delta(t-t')dt, \tag{2.2}$$

where $\langle - \rangle$ denotes the expectation value. The mobility and diffusivity matrices $M = (M^{ab})$ and $D = (D^{ab})$ occurring above are assumed positive and $\boldsymbol{x}$-independent (the latter assumption is for the sake of simplicity and could be relaxed at the cost of few corrective terms). To assure that the noise models the thermal environment at absolute temperature T, we impose the Einstein relation

$$D = k_B T M, \tag{2.3}$$

where k_B is the Boltzmann constant. Potentials $U_t(\boldsymbol{x}) \equiv U(t,\boldsymbol{x})$ are assumed to be sufficiently confining so that the solutions of the stochastic equation (2.1) do not explode in finite time. Given a probability density $\rho_i(\boldsymbol{x})$ at the initial time $t = 0$, such solutions define then for $t \geq 0$ a, in general non-stationary, Markov diffusion process $\boldsymbol{x}(t)$. The instantaneous distributions of the process, describing its statistical properties at fixed times, are given by the probability densities

$$\rho(t,\boldsymbol{x}) = \left\langle \delta(\boldsymbol{x} - \boldsymbol{x}(t))\right\rangle \equiv \exp\left[-\frac{R(t,\boldsymbol{x})}{k_B T}\right], \tag{2.4}$$

that we assume smooth, positive, and with finite moments. They evolve according to the Fokker-Planck equation that may be rewritten as the advection equation

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v}) = 0 \tag{2.5}$$

in the deterministic velocity field

$$\boldsymbol{v}(t,\boldsymbol{x}) = -M\left(\nabla U + k_B T \rho^{-1}\nabla\rho\right)(t,\boldsymbol{x}) = -M\nabla(U-R)(t,\boldsymbol{x}). \tag{2.6}$$

The time-dependent vector field $\boldsymbol{v}(t,\boldsymbol{x})$, called current velocity in [47], has the interpretation of the mean local velocity of the process $\boldsymbol{x}(t)$ defined by the limiting procedure

$$\boldsymbol{v}(t,\boldsymbol{x}) = \lim_{\epsilon\to 0} \frac{\langle \delta(\boldsymbol{x} - \boldsymbol{x}(t))(\boldsymbol{x}(t+\epsilon) - \boldsymbol{x}(t-\epsilon))\rangle}{2\epsilon\langle\delta(\boldsymbol{x}-\boldsymbol{x}(t))\rangle} \tag{2.7}$$

(the limit has to be taken after the expectation as the trajectories of the diffusion process are not differentiable).

The setup of Langevin equation permits simple definitions of thermodynamical quantities. The fluctuating (i.e. trajectory-dependent) work performed on the system between initial time $t = 0$ and final time $t = t_f$ is given by the Jarzynski expression [32]

$$W = \int_0^{t_f} \partial_t U\left(t,\boldsymbol{x}(t)\right)dt \tag{2.8}$$

and the fluctuating heat released into the environment during the same time interval by the formula

$$Q = -\int_0^{t_f} \nabla U\left(t,\boldsymbol{x}(t)\right)\cdot \circ d\boldsymbol{x}(t) \tag{2.9}$$

with the Stratonovich stochastic integral (symbolized by "$\circ$"). The conservation of energy takes the form of the identity

$$W - Q = \int_0^{t_f} \frac{d}{dt} U\big(t, \boldsymbol{x}(t)\big) dt = \Delta U \tag{2.10}$$

following from the rules of the Stratonovich differential calculus, where

$$\Delta U = U\big(t_f, \boldsymbol{x}(t_f)\big) - U\big(0, \boldsymbol{x}(0)\big) \tag{2.11}$$

is the difference of the potential energy between the end points of the process trajectory. Equation (2.10) holds for the fluctuating quantities and implies the relation

$$\langle W \rangle - \langle Q \rangle = \langle \Delta U \rangle \tag{2.12}$$

for the expectation values which is the First Law of Stochastic Thermodynamics. The expectation value of work is given by the identity

$$\langle W \rangle = \int_0^{t_f} dt \int \partial_t U(t, \boldsymbol{x}) \rho(t, \boldsymbol{x}) dx, \tag{2.13}$$

where dx denotes the standard d-dimensional volume element. Since

$$\langle \Delta U \rangle = \int_0^{t_f} dt \int \partial_t \big[U(t, \boldsymbol{x}) \rho(t, \boldsymbol{x}) \big] dx, \tag{2.14}$$

the expectation value of heat release may be easily obtained from identity (2.12):

$$\begin{aligned} \langle Q \rangle &= -\int_0^{t_f} dt \int U(t, \boldsymbol{x}) \partial_t \rho(t, \boldsymbol{x}) dx \\ &= -\int_0^{t_f} dt \int \nabla U(t, \boldsymbol{x}) \cdot \boldsymbol{v}(t, \boldsymbol{x}) \rho(t, \boldsymbol{x}) dx, \end{aligned} \tag{2.15}$$

where we used the advection equation (2.5) and the integration by parts (here and below, we assume that the spatial boundary terms in integration by parts vanish; this is assured for confining potentials and fast decaying initial density of the process).

Let us pass to the discussion of the Second Law of Thermodynamics in the context of Langevin dynamics (2.1). The instantaneous entropy of the system is given by the usual Gibbs-Shannon formula

$$S_{sys}(t) = -k_B \int \ln\big(\rho(t, \boldsymbol{x})\big) \rho(t, \boldsymbol{x}) dx. \tag{2.16}$$

For its time derivative, one obtains, using the Fokker-Planck equation in the form (2.5) and integrating by parts, the expression

$$\begin{aligned} \dot{S}_{sys}(t) &= -k_B \int \big(1 + \ln\big(\rho(t, \boldsymbol{x})\big)\big) \partial_t \rho(t, \boldsymbol{x}) dx \\ &= \frac{1}{T} \int (\nabla R)(t, \boldsymbol{x}) \cdot \boldsymbol{v}(t, \boldsymbol{x}) \rho(t, \boldsymbol{x}) dx. \end{aligned} \tag{2.17}$$

Upon integrating over time, this gives for the change of the entropy of the system in the time interval $[0, t_f]$ the formula

$$\begin{aligned} \Delta S_{sys} &\equiv S_{sys}(t_f) - S_{sys}(0) \\ &= \frac{1}{T} \int_0^{t_f} dt \int (\nabla R)(t, \boldsymbol{x}) \cdot \boldsymbol{v}(t, \boldsymbol{x}) \rho(t, \boldsymbol{x}) dx. \end{aligned} \tag{2.18}$$

Since the system evolves interacting with the thermal environment, the entropy of the latter also changes. The change of entropy of environment is related to the average heat release by the thermodynamical formula

$$\Delta S_{env} = \frac{1}{T}\langle Q \rangle. \tag{2.19}$$

For the total entropy production, Eqs. (2.15) and (2.18) give

$$\begin{aligned}\Delta S_{tot} &= \Delta S_{sys} + \Delta S_{env} \\ &= \frac{1}{T}\int_0^{t_f} dt \int (-\nabla U + \nabla R)(t,\boldsymbol{x}) \cdot \boldsymbol{v}(t,\boldsymbol{x})\rho(t,\boldsymbol{x})dx \\ &= \frac{1}{T}\int_0^{t_f} dt \int \big(\boldsymbol{v} \cdot M^{-1}\boldsymbol{v}\big)(t,\boldsymbol{x})\rho(t,\boldsymbol{x})dx,\end{aligned} \tag{2.20}$$

where in the last line, we used the expression (2.6) for the mean local velocity. Similar formulae for the entropy production appeared e.g. in [4, 16, 41, 51]. In the obvious way, identity (2.20) implies the Second Law of Stochastic Thermodynamics:

$$\Delta S_{tot} \geq 0 \tag{2.21}$$

stating that the total entropy production composed of the changes of entropy of the system and of the environment has to be non-negative. Inequality (2.21) may be also rewritten as a lower bound for the average heat release:

$$\langle Q \rangle \geq -T\Delta S_{sys}. \tag{2.22}$$

3 Landauer Principle

In the form (2.22), the Second Law of Stochastic Thermodynamics is closely related to the Landauer principle [8, 38] stating that the erasure of one bit of information during a computation process conducted in thermal environment requires a release of heat equal (in average) to at least $(\ln 2)k_B T$, see also recent discussions of the relation between the Second Law and information processing in [2, 17, 18, 37, 45, 56]. As an example, consider a bi-stable system that may be in two distinct states and undergoes a process that at final time leaves it always in, say, the second of those states. Such a device may be realized in the context of Stochastic Thermodynamics by an appropriately designed Langevin evolution that starts from the Gibbs state corresponding to a potential with two symmetric wells separated by a high barrier and ends in a Gibbs state corresponding to a potential with only one of those wells. The change of system entropy in such a process is approximately

$$\Delta S_{sys} = -(\ln 1)k_B + 2\left(\ln\frac{1}{2}\right)\frac{1}{2}k_B = -(\ln 2)k_B \tag{3.1}$$

and Landauer's lower bound for average heat release follows from inequality (2.22). Note that in this situation we fix the initial and the final state of Langevin evolution, inquiring how much heat is released during a process that interpolates between those states. As is well known, in order to saturate the lower bounds (2.21) or (2.22), one has to move very slowly in a quasi-stationary way so that the system passes at intermediate times through a sequence of nearly-equilibrium states. Suppose however, that we cannot afford to go too slowly. Indeed, in computational devices, we are interested in fast dynamics that arrives at the final state quickly but produces as little heat as possible. We are therefore naturally led to two questions:

- What is the lower bound for the total entropy production or the average heat release in the process that interpolates between given states in a time interval of fixed length?
- What is the dynamical protocol that leads to such a minimal total entropy production or heat release?

These questions make sense in a variety of setups. They are among the core ones of the so-called Finite-Time Thermodynamics [1, 14] that was developed during last decades mostly with an eye on technological applications. Here we shall study them in the framework of Stochastic Thermodynamics of processes described by Langevin equation (2.1). The initial and final states will be given by probability densities $\rho_i(\boldsymbol{x}) = \rho(0, \boldsymbol{x})$ and $\rho_f(\boldsymbol{x}) = \rho(t_f, \boldsymbol{x})$. The dynamical protocols will be determined by specifying for $0 \leq t \leq t_f$ a time dependent steering potential $U(t, \boldsymbol{x})$, that will be called the "control" below. In such a setup, the question about the minimum of total entropy production or average heat release becomes an optimization problem in Control Theory [22, 29]. It was recently discussed, together with the optimization of average performed work, in Refs. [3, 48], see also [4, 28].

4 Optimal Control of Entropy Production

We shall describe below a relation of the minimization problem for total entropy production or the average heat release to the optimal mass transport [55] and the inviscid Burgers dynamics [13]. To our knowledge, such a relation was first established in Ref. [3] using stochastic optimization. Nevertheless, connections between stochastic control and (viscous) Burgers equation and between Fokker-Planck equation and optimal mass transport are old themes, see e.g. Chap. VI of [22], or [31] in a particular case, for the first ones and [34] for the second ones. Here, inspired by the discussion in [4], we shall minimize the total entropy production given by Eq. (2.20) by a direct argument in the spirit of deterministic optimal control.

Our strategy is based on the subsequent use of the obvious fact that if a minimizer of a function on a bigger set lies in a smaller one then it realizes also the minimum of the function over the smaller set. We shall minimize the functional

$$\mathcal{A}[\boldsymbol{v}, \rho_i] = \int_0^{t_f} dt \int \big(\boldsymbol{v} \cdot M^{-1}\boldsymbol{v}\big)(t, \boldsymbol{x})\rho(t, \boldsymbol{x})dx, \tag{4.1}$$

where $\rho(t, \boldsymbol{x})$ is determined by the advection equation (2.5) from the initial density ρ_i and the velocity field $\boldsymbol{v}(t, \boldsymbol{x})$, over all velocity fields $\boldsymbol{v}$ under the constraint that $\rho(t_f, \boldsymbol{x}) = \rho_f(\boldsymbol{x})$. Such an extended minimization problem was considered in [6]. The crucial but simple additional step will be the observation that the optimal velocity field $\boldsymbol{v}(t, \boldsymbol{x})$ for which the constraint minimum is attained is a local mean velocity for a certain control $U(t, \boldsymbol{x})$. The latter realizes then the Langevin dynamics that interpolates on the time interval $[0, t_f]$ between densities ρ_i and ρ_f with minimal total entropy production ΔS_{tot}.

In [6], see also [7], it was shown how one may reduce the constraint minimization of functional (4.1) to the optimal mass transport problem. Here is a slight modification of that argument. We shall admit smooth velocity fields $\boldsymbol{v}$ for which the Lagrangian trajectories $\boldsymbol{x}(t)$ solving the equation

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{v}\big(t, \boldsymbol{x}(t)\big), \tag{4.2}$$

where the dot stands for t-derivative, do not blow up. E.g., we may take $\boldsymbol{v}$ bounded by a linear function of $|\boldsymbol{x}|$. The solution of the advection equation (2.5) is then given by the formula

$$\rho(t, \boldsymbol{x}) = \int \delta\big(\boldsymbol{x} - \boldsymbol{x}(t; \boldsymbol{x}_i)\big)\rho_i(\boldsymbol{x}_i)dx_i, \tag{4.3}$$

where $\boldsymbol{x}(t;\boldsymbol{x}_i)$ denotes the Lagrangian trajectory that passes through $\boldsymbol{x}_i$ at time $t=0$. The substitution of Eq. (4.3) into definition (4.1) results in the identity

$$\mathcal{A}[\boldsymbol{v},\rho_i]=\int_0^{t_f}dt\int\dot{\boldsymbol{x}}(t;\boldsymbol{x}_i)\cdot M^{-1}\dot{\boldsymbol{x}}(t;\boldsymbol{x}_i)\rho_i(\boldsymbol{x}_i)d\boldsymbol{x}_i. \tag{4.4}$$

Since velocity field $\boldsymbol{v}(t,\boldsymbol{x})$ may be recovered from its Lagrangian flow $\boldsymbol{x}(t;\boldsymbol{x}_i)$, the minimization of $\mathcal{A}[\boldsymbol{v},\rho_i]$ over velocity fields may be replaced by the minimization of the right hand side of (4.4) over Lagrangian flows such that the map $\boldsymbol{x}_i\mapsto\boldsymbol{x}(t_f;\boldsymbol{x}_i)\equiv\boldsymbol{x}_f(\boldsymbol{x}_i)$ is constrained by the condition

$$\rho_f(\boldsymbol{x})=\int\delta\big(\boldsymbol{x}-\boldsymbol{x}_f(\boldsymbol{x}_i)\big)\rho_i(\boldsymbol{x}_i)d\boldsymbol{x}_i, \tag{4.5}$$

or, equivalently, denoting by $\frac{\partial(\boldsymbol{x}_f(\boldsymbol{x}_i))}{\partial(\boldsymbol{x}_i)}$ the Jacobian of the map $\boldsymbol{x}_i\mapsto\boldsymbol{x}_f(\boldsymbol{x}_i)$, by the requirement that

$$\rho_f\big(\boldsymbol{x}_f(\boldsymbol{x}_i)\big)\frac{\partial(\boldsymbol{x}_f(\boldsymbol{x}_i))}{\partial(\boldsymbol{x}_i)}=\rho_i(\boldsymbol{x}_i). \tag{4.6}$$

In other words, the Lagrangian map $\boldsymbol{x}_i\mapsto\boldsymbol{x}_f(\boldsymbol{x}_i)$ should transport the initial density ρ_i into the final one ρ_f. Upon exchange of the order of integration, the minimization of functional (4.4) may be done in three steps:

- First, we fix a smooth Lagrangian map

$$\boldsymbol{x}_i\mapsto\boldsymbol{x}_f(\boldsymbol{x}_i) \tag{4.7}$$

  with a smooth inverse $\boldsymbol{x}_f\mapsto\boldsymbol{x}_i(\boldsymbol{x}_f)$ such that constraint (4.6) holds.
- Second, for each $\boldsymbol{x}_i$, we minimize

$$\int_0^{t_f}\dot{\boldsymbol{x}}(t;\boldsymbol{x}_i)\cdot M^{-1}\dot{\boldsymbol{x}}(t;\boldsymbol{x}_i)dt \tag{4.8}$$

  over the curves $[0,t_f]\ni t\mapsto\boldsymbol{x}(t;\boldsymbol{x}_i)$ starting from $\boldsymbol{x}_i$ and ending at $\boldsymbol{x}_f(\boldsymbol{x}_i)$. Due to the positivity of matrix M, the minimal curves are just the straight lines

$$[0,t_f]\ni t\mapsto\boldsymbol{x}(t;\boldsymbol{x}_i)=\frac{t_f-t}{t_f}\boldsymbol{x}_i+\frac{t}{t_f}\boldsymbol{x}_f(\boldsymbol{x}_i) \tag{4.9}$$

  with constant time-derivative $\dot{\boldsymbol{x}}(t;\boldsymbol{x}_i)=(\boldsymbol{x}_f(\boldsymbol{x}_i)-\boldsymbol{x}_i)/t_f$.
- Third, we minimize the "quadratic cost functional"

$$\mathcal{K}\big[\boldsymbol{x}_f(\cdot)\big]=\int\big(\boldsymbol{x}_f(x_i)-\boldsymbol{x}_i\big)\cdot M^{-1}\big(\boldsymbol{x}_f(x_i)-\boldsymbol{x}_i\big)\rho_i(\boldsymbol{x}_i)dx_i \tag{4.10}$$

  over the maps $\boldsymbol{x}_i\mapsto\boldsymbol{x}_f(\boldsymbol{x}_i)$ satisfying constraint (4.6).

In principle, the above three-step minimization is over a broader class of maps $\boldsymbol{x}(t;\boldsymbol{x}_i)$ which might be non-invertible for fixed intermediate t, not representing the Lagrangian flow of any velocity field $\boldsymbol{v}(t,\boldsymbol{x})$. As we shall see in the next section, however, the minimizer (4.9) represents such a flow if $x_f(\boldsymbol{x}_i)$ minimizes the cost function (4.10) under constraint (4.6).

5 Monge-Kantorovich Mass Transport and Burgers Equation

The minimization of the quadratic cost function (4.10) over invertible Lagrangian maps $\boldsymbol{x}_i\mapsto\boldsymbol{x}_f(\boldsymbol{x}_i)$ satisfying constraint (4.6) is the celebrated Monge-Kantorovich optimal mass

transport problem [36, 44] related to the inviscid Burgers equation [6, 7, 55]. For reader's convenience, we shall briefly recall that relation in the present section.

Observe that constraint (4.6) may be rewritten in the equivalent form in terms of inverse Lagrangian maps as the identity

$$\rho_f(\boldsymbol{x}_f) = \rho_i\big(\boldsymbol{x}_i(\boldsymbol{x}_f)\big)\frac{\partial(\boldsymbol{x}_i(\boldsymbol{x}_f))}{\partial(\boldsymbol{x}_f)}. \tag{5.1}$$

In the latter form, it implies for the infinitesimal variation $\delta\boldsymbol{x}_i(\boldsymbol{x}_f)$ of the inverse Lagrangian map the no-divergence condition

$$\nabla_{\boldsymbol{x}_i} \cdot \big(\rho_i(\boldsymbol{x}_i)\delta\boldsymbol{x}_i\big(\boldsymbol{x}_f(\boldsymbol{x}_i)\big)\big) = 0. \tag{5.2}$$

Changing variables in the expression (4.10) and using constraint (5.1), we may re-express the cost function in an equivalent form involving the final density:

$$\mathcal{K}\big[\boldsymbol{x}_f(\cdot)\big] = \int \big(\boldsymbol{x}_f - \boldsymbol{x}_i(\boldsymbol{x}_f)\big) \cdot M^{-1}\big(\boldsymbol{x}_f - \boldsymbol{x}_i(\boldsymbol{x}_f)\big)\rho_f(\boldsymbol{x}_f)d\boldsymbol{x}_f. \tag{5.3}$$

The variation of the latter is

$$\begin{aligned}\delta\mathcal{K}\big[\boldsymbol{x}_f(\cdot)\big] &= 2\int \big(\boldsymbol{x}_i(\boldsymbol{x}_f) - \boldsymbol{x}_f\big) \cdot M^{-1}\delta\boldsymbol{x}_i(\boldsymbol{x}_f)\rho_f(\boldsymbol{x}_f)d\boldsymbol{x}_f \\ &= 2\int \big(\boldsymbol{x}_i - \boldsymbol{x}_f(\boldsymbol{x}_i)\big) \cdot M^{-1}\delta\boldsymbol{x}_i\big(\boldsymbol{x}_f(\boldsymbol{x}_i)\big)\rho_i(\boldsymbol{x}_i)d\boldsymbol{x}_i.\end{aligned} \tag{5.4}$$

For the extremal maps $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i)$, variation (5.4) has to vanish for all $\delta\boldsymbol{x}_i(\boldsymbol{x}_f(\boldsymbol{x}_i))$ satisfying (5.2). This occurs if and only if $M^{-1}(\boldsymbol{x}_i - \boldsymbol{x}_f(\boldsymbol{x}_i))$ is a gradient, i.e. if there exists a function $F(\boldsymbol{x}_i)$ such that

$$\boldsymbol{x}_f(\boldsymbol{x}_i) = M\nabla F(\boldsymbol{x}_i). \tag{5.5}$$

Substituting this relation to expression (4.6) for the constraint one infers that function F solves the Monge-Ampère equation

$$\rho_f\big(M\nabla F(\boldsymbol{x}_i)\big)\det\left(M^{ac}\frac{\partial^2 F}{\partial x_i^b \partial x_i^c}(\boldsymbol{x}_i)\right) = \rho_i(\boldsymbol{x}_i) \tag{5.6}$$

and, in particular, that

$$\det\left(M^{ac}\frac{\partial^2 F}{\partial x_i^b \partial x_i^c}(\boldsymbol{x}_i)\right) > 0 \tag{5.7}$$

(in the above relations, the mobility matrix M may be absorbed by the linear change of variables $\boldsymbol{x} \mapsto \boldsymbol{x}' = \sqrt{M}\boldsymbol{x}$). The crucial input from the theory of Monge-Kantorovich optimal mass transport is the result that the minimizer $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i)$ of the cost function exists and is the unique extremum corresponding to a function F which is convex [25, 55]. Note that it follows then from Eq. (5.7) that the Hessian matrix of F is everywhere strictly positive. Now, interpolating between $\frac{1}{2}\boldsymbol{x}_i \cdot M^{-1}\boldsymbol{x}_i$ and function $F(\boldsymbol{x}_i)$, set

$$F_t(\boldsymbol{x}_i) = \frac{t_f - t}{2t_f}\boldsymbol{x}_i \cdot M^{-1}\boldsymbol{x}_i + \frac{t}{t_f}F(\boldsymbol{x}_i) \tag{5.8}$$

for $0 \le t \le t_f$. Hence

$$M\nabla F_t(\boldsymbol{x}_i) = \frac{t_f - t}{t_f}\boldsymbol{x}_i + \frac{t}{t_f}\boldsymbol{x}_f(\boldsymbol{x}_i) = \boldsymbol{x}(t; \boldsymbol{x}_i), \tag{5.9}$$

giving the linear interpolation between $\boldsymbol{x}_i$ and $\boldsymbol{x}_f(\boldsymbol{x}_i)$, just like in (4.9). A little argument shows that the positivity of the Hessian of F implies that the maps $\boldsymbol{x}_i \mapsto \boldsymbol{x}(t;\boldsymbol{x}_i)$ are diffeomorphisms of $\mathbf{R}^d$ for all $t \in [0, t_f]$. It then makes sense to define a function $\Psi(t,\boldsymbol{x})$ by the relation

$$\Psi(t,\boldsymbol{x}) = \frac{1}{t}\left[\frac{1}{2}\boldsymbol{x}\cdot M^{-1}\boldsymbol{x} - \boldsymbol{x}\cdot M^{-1}\boldsymbol{x}_i + F_t(\boldsymbol{x}_i)\right]_{\boldsymbol{x}(t;\boldsymbol{x}_i)=\boldsymbol{x}}. \tag{5.10}$$

Note that the derivative over $\boldsymbol{x}_i$ of the term $[\cdots]$ on the right hand side vanishes for $\boldsymbol{x}(t;\boldsymbol{x}_i) = \boldsymbol{x}$ due to Eq. (5.9). It follows that

$$\begin{aligned} \partial_t\Psi(t,\boldsymbol{x}) &= -\frac{1}{2t^2}(\boldsymbol{x}-\boldsymbol{x}_i)\cdot M^{-1}(\boldsymbol{x}-\boldsymbol{x}_i), \\ \nabla\Psi(t,\boldsymbol{x}) &= \frac{1}{t}M^{-1}(\boldsymbol{x}-\boldsymbol{x}_i) \end{aligned} \tag{5.11}$$

for $\boldsymbol{x}(t;\boldsymbol{x}_i) = \boldsymbol{x}$. Equations (5.9) and (5.11) entail that

$$\begin{aligned} \dot{\boldsymbol{x}}(t;\boldsymbol{x}_i) &= \frac{1}{t_f}\big(\boldsymbol{x}_f(\boldsymbol{x}_i) - \boldsymbol{x}_i\big) = \frac{1}{t}\big(\boldsymbol{x}(t;\boldsymbol{x}_i) - \boldsymbol{x}_i\big) \\ &= M(\nabla\Psi)\big(t,\boldsymbol{x}(t;\boldsymbol{x}_i)\big) = \boldsymbol{v}\big(t,\boldsymbol{x}(t;\boldsymbol{x}_i)\big) \end{aligned} \tag{5.12}$$

so that the interpolating maps $\boldsymbol{x}_i \mapsto \boldsymbol{x}(t;\boldsymbol{x}_i)$ provide the Lagrangian flow of the velocity field

$$\boldsymbol{v}(t,\boldsymbol{x}) = M\nabla\Psi(t,\boldsymbol{x}) \tag{5.13}$$

that is constant along its Lagrangian trajectories $t \mapsto \boldsymbol{x}(t;\boldsymbol{x}_i)$. Such a behavior characterizes velocities solving the inviscid Burgers equation (the Euler equation without pressure)

$$\partial_t\boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} = 0. \tag{5.14}$$

Indeed, as follows from Eqs. (5.11), the velocity potential Ψ satisfies the non-linear evolution equation

$$\partial_t\Psi + \frac{1}{2}(\nabla\Psi)\cdot M(\nabla\Psi) = 0 \tag{5.15}$$

which implies the Burgers equation (5.13).

Let us define the intermediate densities $\rho(t,\boldsymbol{x})$ that interpolate over the time interval $[0, t_f]$ between ρ_i and ρ_f by Eq. (4.3) so that they evolve according to the advection equation (2.5) in the Burgers velocity field $\boldsymbol{v}$ of Eq. (5.13). It is the assumption that the initial and final densities are smooth that assures that such velocities do not involve shocks on the time interval $[0, t_f]$.

Summarizing the above discussion, we infer that the Burgers velocity field $v(t,\boldsymbol{x})$ of Eq. (5.13), together with the densities $\rho(t,\boldsymbol{x})$ of Eq. (4.3), minimize functional $\mathcal{A}[\boldsymbol{v},\rho_i]$ of Eq. (4.1) over the space of velocities $\boldsymbol{v}(t,\boldsymbol{x})$ and densities $\rho(t,\boldsymbol{x})$ that evolve for $0 \le t \le t_f$ by the advection equation (2.5) interpolating between ρ_i and ρ_f. The minimal value of functional $\mathcal{A}[\boldsymbol{v},\rho_i]$ under the above constraint is

$$\mathcal{A}_{min} = \frac{1}{t_f}\mathcal{K}_{min}, \tag{5.16}$$

where $\mathcal{K}_{min}$ is the value of the quadratic cost function (4.10) on the minimizer $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(x_i)$. These are the main results of [6, 7], see also Chap. 8 of [55] for more details. That $\mathcal{A}_{min}$ had to be inversely proportional to the length of the time interval could have been inferred directly by rescaling of time in functional (4.1) [49].

Below, we shall use the following factorization property of the optimal mass transport problem with the cost function (4.10) holding if the mobility matrix has the block form

$$M = \begin{pmatrix} M^1 & 0 \\ 0 & M^2 \end{pmatrix}. \tag{5.17}$$

If, with respect to the corresponding decomposition of the d-dimensional space, both initial and final densities have the product form:

$$\rho_i(\boldsymbol{x}) = \rho_i^1(\boldsymbol{x}^1)\rho_i^2(\boldsymbol{x}^2), \qquad \rho_f(\boldsymbol{x}) = \rho_f^1(\boldsymbol{x}^1)\rho_f^2(\boldsymbol{x}^2) \tag{5.18}$$

for $\boldsymbol{x} = (\boldsymbol{x}^1, \boldsymbol{x}^2)$, then the Lagrangian map minimizing cost function (4.10) also factorizes into the product of minimizers of the lower dimensional problems:

$$\begin{aligned} \boldsymbol{x}_f(\boldsymbol{x}_i) &= M\nabla F(\boldsymbol{x}_i) = \left(\boldsymbol{x}_f^1(\boldsymbol{x}_i^1), \boldsymbol{x}_f^2(\boldsymbol{x}_i^1)\right) \\ &= \left(M^1\nabla F^1(\boldsymbol{x}_i^1), M^2\nabla F^2(\boldsymbol{x}_i^2)\right) \end{aligned} \tag{5.19}$$

and the minimal cost is the sum of the lower-dimensional ones. This follows from the uniqueness of the minimizer and its characterization in terms of the gradient of a convex function. The corresponding Burgers potential $\Psi(t, \boldsymbol{x})$ is then the sum, and the interpolating density $\rho(t, \boldsymbol{x})$ the product, of the ones obtained from the lower dimensional minimizers.

6 Second Law of Stochastic Thermodynamics at Short Times

Let us denote by $R(t, \boldsymbol{x})$ the dynamical potential related by Eq. (2.4) to the optimal densities $\rho(t, \boldsymbol{x})$ given by Eq. (4.3). Set

$$U(t, \boldsymbol{x}) = R(t, \boldsymbol{x}) - \Psi(t, \boldsymbol{x}), \tag{6.1}$$

where Ψ is the Burgers potential (5.10). Equation (5.13) for the optimal velocity may be rewritten as

$$\boldsymbol{v} = M\nabla(R - U), \tag{6.2}$$

meaning that $\boldsymbol{v}$ is the mean local velocity of the overdamped Langevin process with control U. We infer that the optimal ρ evolving by the advection equation (2.5), describes the instantaneous probability densities of such a process with initial values distributed with density ρ_i. It follows then from relation (2.20) that control U provides the optimal protocol on the time interval $[0, t_f]$ that under the Langevin dynamics (2.1) evolves the initial state ρ_i to the final state ρ_f with the minimal total entropy production equal to $\frac{1}{T}\mathcal{A}_{min}$ for $\mathcal{A}_{min}$ given by Eq. (5.16). We obtain this way a refinement for finite time intervals of the Second Law (2.21) of Stochastic Thermodynamics:

Theorem *For the Langevin dynamics* (2.1) *on the time interval* $[0, t_f]$ *that evolves between states* ρ_i *and* ρ_f,

$$\Delta S_{tot} \geq \frac{1}{t_f T}\mathcal{K}_{min}, \tag{6.3}$$

with the inequality saturated by the optimal evolution with the time dependent potential $U(t, \boldsymbol{x})$ *constructed above.*

Here, as in relation (2.21), $\Delta S_{tot} = \Delta S_{sys} + \Delta S_{env}$ denotes the total entropy change, composed of the change of entropy of the system ΔS_{sys} and the change of entropy of the thermal environment $\Delta S_{env} = \frac{1}{T}\langle Q\rangle$ during the process. The theorem states that the total change of entropy during Langevin evolution (2.1) is not smaller than the minimal quadratic cost function (involving the mobility matrix M) for the deterministic transport of initial probability distribution to the final one, divided by the product of time length t_f of the process by temperature T of the environment. Since the cost function is strictly positive whenever the initial and final probability distributions are different, it follows that the shorter the time length of the process and the smaller temperature, the bigger minimal total entropy production. The latter may approach zero only for (adiabatically slow) processes taking very long time. Inequality (6.3) provides then a quantitative refinement of the Second Law of Stochastic Thermodynamics (2.21) for processes whose time span does not exceed t_f. In order to determine the optimal protocol $U(t, \boldsymbol{x})$ of Eq. (6.1), one has to find subsequently:

1. the minimizer $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i) = M\nabla F(\boldsymbol{x}_i)$ of the cost function of Eq. (4.10) under the constraint (4.6) such that $\mathcal{K}_{min} = \mathcal{K}[\boldsymbol{x}_f(\cdot)]$;
2. the solution Ψ given by Eq. (5.10) of the Burgers equation (5.15) for potentials;
3. the solution ρ given by Eq. (4.3) of the advection equation (2.5) in the Burgers velocity field $\boldsymbol{v} = M\nabla\Psi$.

The refined Second Law (6.3) may be rewritten as a refinement of the lower bound (2.22) for the heat release in processes with fixed initial and final densities that takes the form

$$\langle Q\rangle \geq \frac{1}{t_f}\mathcal{K}_{min} - T\Delta S_{sys}, \tag{6.4}$$

and is saturated for the same optimal protocol that the inequality (6.3). Clearly, the refinements (6.3) or (6.4) become relevant for times

$$t_f \lesssim \frac{\mathcal{K}_{min}}{T|\Delta S_{sys}|}, \tag{6.5}$$

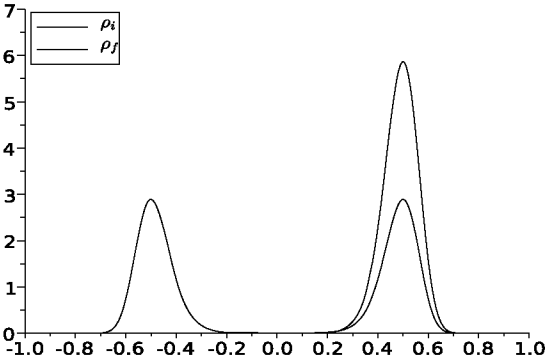
where the right hand sets a time scale depending on the mobility and the limiting states of the system as well as on the temperature of the environment. One may view this time scale as setting divide between fast and slow processes. An illustration of the above results is provided by the case of Gaussian processes first considered in [48] and generalized in [3]. The initial and final distributions, as well as the optimal ones at intermediate times are Gaussian in that example and the optimal control potential stays quadratic. The main lesson of those examples was that initial and final values of the optimal control are different from the potentials that, when frozen in time, would have, respectively, the initial and the final densities as the invariant Gibbs states. This is a general phenomenon because the initial and the final values of the Burgers potential $\Psi = R - U$ for the optimal protocol are non-constant if $\rho_i \neq \rho_f$ since, by the second of Eqs. (5.11),

$$\begin{aligned}(\nabla\Psi)(0, \boldsymbol{x}_i) &= \frac{1}{t_f}M^{-1}\big(\boldsymbol{x}_f(\boldsymbol{x}_i) - \boldsymbol{x}_i\big),\\ \nabla\Psi(t_f, \boldsymbol{x}_f) &= \frac{1}{t_f}M^{-1}\big(\boldsymbol{x}_f - \boldsymbol{x}_i(\boldsymbol{x}_f)\big).\end{aligned} \tag{6.6}$$

7 Finite Time Refinement of Landauer Principle

The finite time refinement (6.4) of the lower bound (2.22) for the average heat release implies immediately a refinement of the Landauer bound for the average heat dissipated during

Fig. 1 ρ_i and ρ_f



the memory erasure of one bit of information in Langevin processes for which such erasure is related to the change $\Delta S_{sys} = -(\ln 2)k_B$ of the entropy of the system, see Sect. 2. The improved bound takes the form

$$\langle Q \rangle \geq \frac{1}{t_f}\mathcal{K}_{min} + (\ln 2)k_B T, \tag{7.1}$$

where $\mathcal{K}_{min}$ is the minimal value of the cost function (4.10). In [17], the distribution of the released heat (and work) was studied numerically for a particular memory erasure overdamped one-dimensional Langevin dynamics. It was checked that the mean heat release $\langle Q \rangle$ satisfied the Landauer bound, but that, with small but sizable probability, the fluctuating values of Q may violate the bound. In [10], heat release was studied in an experimental realization of a similar system undergoing a memory erasure dynamics. In the experiment, a silica ball with diameter of 2 μm suspended in a flat horizontal cell with ultra pure water at room temperature was manipulated by laser tweezers in order to displace the ball localized initially in a double trap to a fixed one of two traps. It was noticed in [10] (in Fig. 3c) that, for a specific dynamical protocol, the difference between the mean heat release and the Landauer lower bound decreased with the time length t_f of the erasure process (the decrease seemed inversely proportional to t_f for long times). In order to see how the optimal protocol for which the upper bound in (7.1) is saturated looks like in the experimental situation, we considered a 1-dimensional stochastic evolution (2.1) with mobility $\mu = \frac{0.213877}{k_B T}\frac{\mu m^2}{s}$ and the limiting distributions

$$\rho_i(x) = \frac{1}{Z_i}\exp\left[-\frac{A}{k_B T}\left(x^2-\alpha^2\right)^2\right] \equiv \exp\left[-\frac{1}{k_B T}R_i(x)\right], \tag{7.2}$$

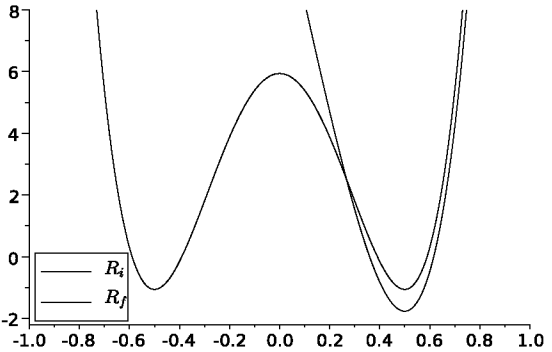
$$\rho_f(x) = \frac{1}{Z_f}\exp\left[-\frac{A}{k_B T}(x-\alpha)^2\left((x-\alpha)^2+3\alpha(x-\alpha)+4\alpha^2\right)\right]$$
$$\equiv \exp\left[-\frac{1}{k_B T}R_f(x)\right], \tag{7.3}$$

for $A = 112 k_B T\ \mu m^{-4}$, $\alpha = 0.5$ μm, and x expressed in μm's, see Figs. 1 and 2. The entropy difference between ρ_i and ρ_f is

$$\Delta S \approx -0.74312 k_B \tag{7.4}$$

which is equal to $-(\ln 2)k_B$ within 7.3 %.

Fig. 2 R_i and R_f



The experimental situation is close to a two-dimensional one in the horizontal plane, where the above initial and final densities in the direction of x-axis are multiplied by the same density

$$\rho(y) = \frac{1}{Z} \exp\left[-\frac{A}{k_B T} y^2 \left(y^2 + 4\alpha^2\right)\right] \tag{7.5}$$

in the direction of y-axis, leading to the same entropy difference (7.4). In such a two-dimensional situation, however, the Lagrangian map for the optimal mass transport factorizes into the map $x_i \mapsto x_f(x_i)$ giving the optimal transport of $\rho_i(x)$ to $\rho_f(x)$ times the identity map in the y-direction, see the end of Sect. 5. The minimal cost for the 2-dimensional problem coincides then with the one for the map $x_f(x_i)$. The corresponding two-dimensional optimal control is the sum of the optimal control $U(t, x)$ for the one-dimensional problem in the x-direction and of the static potential $U(y) = Ay^2(y^2 + 4\alpha^2 y^2)$. Consequently, the two-dimensional problem reduces to the one-dimensional one in the direction of the x-axis. Similarly, the strong confining potential in the vertical z-direction may be ignored as long as it is x- and y-independent.

We employed three methods to find the optimal Lagrangian map $x_i \mapsto x_f(x_i)$ that transports ρ_i to ρ_f and minimizes the quadratic cost. First, the unique positively oriented map $x_i \mapsto x_f(x_i)$ that transports ρ_i to ρ_f may be found from the relation

$$\int_{-\infty}^{x_f(x_i)} \rho_f(x)dx = \int_{-\infty}^{x_i} \rho_i(x)dx. \tag{7.6}$$

According to the general theory exposed in Sect. 5, it has to minimize the quadratic cost since it is a gradient of a convex function. We solve Eq. (7.6) for $x_f(x_i)$ numerically in Scilab, using the *fsolve* procedure, for discrete values of x_i spaced by 5 nm lying in the interval $-0.7725\ \mu\text{m} \leq x_i \leq 0.6925\ \mu\text{m}$. This method did not give access to the remaining values of x_i, the numbers involved exceeding there the program capacity. Instead, for $x_i < -0.7725\ \mu\text{m}$, the Lagrangian map $x_i \mapsto x_f(x_i)$ was calculated by expanding $(x_f(x_i) - x_i)$ in powers of $(x_i - \alpha)^{-1}$ up to order 11. The coefficients of the expansion were found from the derivative equation

$$\frac{dx_f(x_i)}{dx_i} = \frac{\rho_i(x_i)}{\rho_f(x_f(x_i))}. \tag{7.7}$$

Similarly, for $x > 0.6925\ \mu\text{m}$, the map $x_i \mapsto x_f(x_i)$ was computed by expanding $(x_f(x_i) - x_i)$ in powers of $(x_i + \alpha)^{-1}$. Finally, in order to check the above results, in particular around the boundary points of the x_i-intervals, where they become less reliable, we performed numerical search for the solution of the corresponding optimal assignment problem, usually

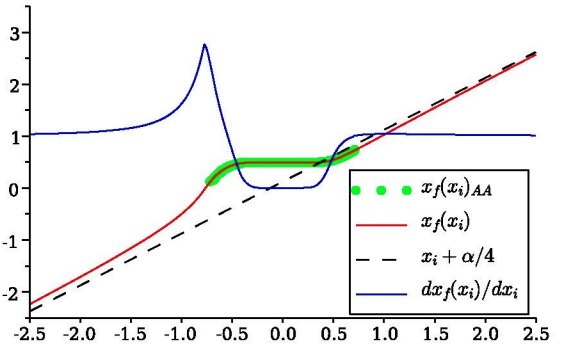


Fig. 3 Lagrangian map $x_f(x_i)$, its asymptotes and its derivative

employed in numerical optimization of higher-dimensional mass transport [11]. The task is to find the permutation π of length N that induces a bijective map $\boldsymbol{q}_n \mapsto \boldsymbol{x}_{\pi(n)}$ between N points ("particles") $\boldsymbol{q}_n$ distributed with density ρ_i and N points $\boldsymbol{x}_n$ distributed with density ρ_f, minimizing the discretized quadratic cost

$$\mathcal{K}_N = \sum_{n=1}^{N} (\boldsymbol{x}_{\pi(n)} - \boldsymbol{q}_n) \cdot M^{-1} (\boldsymbol{x}_{\pi(n)} - \boldsymbol{q}_n) \tag{7.8}$$

(usually one takes M equal or proportional to the unit matrix). The optimal assignment $\boldsymbol{q}_n \mapsto \boldsymbol{x}_{\pi(n)}$ gives a discrete approximation to the optimal Lagrangian map $\boldsymbol{x}_i \mapsto \boldsymbol{x}_f(\boldsymbol{x}_i)$. The optimal permutation π may be searched for employing a version of the Auction Algorithm [9], see also Sect. 4 of [11]. In our one-dimensional simulation, we took $N = 10^5$. As an independent check of the method, we also performed the two-dimensional simulations with the factor (7.5) included in the density, confirming the (approximately) factorized form of the resulting optimal assignment. Figure 3 compiles the results for the three methods of computation of the Lagrangian minimizer $x_i \to x_f(x_i)$ (the broken curve $x_i \mapsto x_i + \alpha/4$ is its exact asymptote at $\pm\infty$) and of its derivative. The results agree well in the common domains. The green thick dots represent the assignment obtained with the Auction Algorithm.

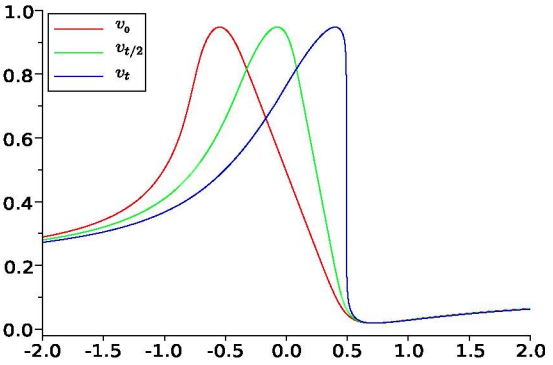
Given the optimal Lagrangian map $x_f(x_i)$, we put the dynamics into it by interpolation defining

$$x(t; x_i) = \frac{t_f - t}{t_f} x_i + \frac{t}{t_f} x_f(x_i). \tag{7.9}$$

The corresponding Burgers velocities

$$v(t, x) = \mu \nabla \Psi(t, x) = \frac{1}{t_f} \big(x_f(x_i) - x_i\big)\Big|_{x(t;x_i)=x} \tag{7.10}$$

for $t_f = 1$ s are plotted in Fig. 4 as function of x at times $t = 0$, $t = t_f/2$, and $t = t_f$. For other process durations the corresponding vertical scale would be divided by t_f. As we see, the evolution of the Burgers velocities that displace the initial distribution to the final one over time t_f describes a nascent shock. The dynamical potentials $R_t = -k_B T \ln \rho_t$ and the time-dependent optimal controls U_t are drawn on Fig. 5 for $t_f = 1$ s (left figure) and for $t_f = 10$ s (right figure). Note that for $t_f = 1$ s, the initial control U_0 is quite different from $R_i = R_0$, rearranging the symmetric wells by making the right one deeper. The half-time control $U_{t_f/2}$ moves the left metastable well further to the right. In the final control U_{t_f}, the



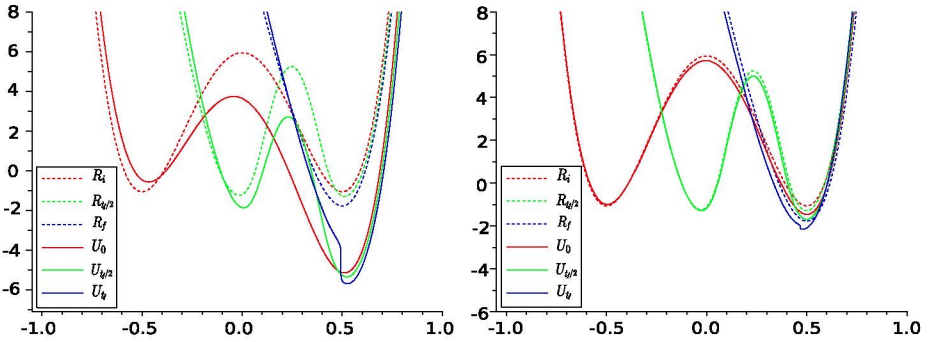


Fig. 4 Burgers velocity at initial, half-time and final time for $t_f = 1$ s

Fig. 5 Initial, half-time and final potentials (*pointed curves*) and initial, half-time and final controls (*solid curves*) for $t_f = 1$ s (*left figure*) and $t_f = 10$ s (*right figure*)

left well disappears altogether. On the other hand, for $t_f = 10$ s, controls U_i become close to dynamical potentials R_t (U_t would coincide with R_t for an infinitely slow process).

The quadratic cost function corresponding to the optimal Lagrangian map $x_i \mapsto x_f(x_i)$

$$\frac{1}{k_B T}\mathcal{K}_{min} \approx 1.996 \text{ s} \tag{7.11}$$

(the Auction Algorithm produced a value lower by 0.07 %, giving an idea about the accuracy of our calculations). The minimal average heat release during the process with duration $t_f = 1$ s is

$$\langle Q \rangle_{min}^{t_f = 1 \text{ s}} \approx (1.996/1 + 0.743) k_B T = 2.739 k_B T \tag{7.12}$$

whereas for the 10 times longer process

$$\langle Q \rangle_{min}^{t_f = 10 \text{ s}} \approx (1.996/10 + 0.7431204) k_B T \approx 0.943 k_B T. \tag{7.13}$$

The average heat release exceeds the Landauer bound $(\ln 2) k_B T \approx 0.693 k_B T$ almost 4 times in the first case and by about 36 % in the second one. The time scale (6.5) on which the extra term in the refinement (7.1) of the Landauer bound becomes important is about 2.7 s in the above model.

8 Extension to Non-conservative Forces

The overdamped Langevin dynamics (2.1) has the drift given by the gradient of a potential. In the presence of non-conservative forces, the corresponding stochastic equation should be modified to

$$d\boldsymbol{x} = M\big(-\nabla U(t,\boldsymbol{x}) + \boldsymbol{f}(t,\boldsymbol{x})\big)dt + d\boldsymbol{\zeta}(t), \tag{8.1}$$

where $\boldsymbol{f}$ represents such forces. We shall keep the noise as before assuming that the environment is still thermal and the Einstein relation (2.3) holds. Equation (8.1) defines again a Markov diffusion process $\boldsymbol{x}(t)$. The Fokker-Planck equation describing the evolution of its instantaneous probability densities $\rho(t,\boldsymbol{x})$ still takes the form of the advection equation (2.5) in the mean local velocity field (2.7) that becomes

$$\begin{aligned}\boldsymbol{v}(t,\boldsymbol{x}) &= -M\big(\nabla U - \boldsymbol{f} + k_B T \rho^{-1}\nabla\rho\big)(t,\boldsymbol{x})\\ &= -M(\nabla U - \boldsymbol{f} - \nabla R)(t,\boldsymbol{x}).\end{aligned} \tag{8.2}$$

The fluctuating heat release is now given by a generalization of formula (2.9):

$$Q = \int_0^{t_f} \big(-\nabla U\big(t,\boldsymbol{x}(t)\big) + \boldsymbol{f}\big(t,\boldsymbol{x}(t)\big)\big)\cdot \circ d\boldsymbol{x}(t), \tag{8.3}$$

with the expectation value

$$\langle Q\rangle = -\int_0^{t_f} dt \int (\nabla U - \boldsymbol{f})(t,\boldsymbol{x})\cdot \boldsymbol{v}(t,\boldsymbol{x})\rho(t,\boldsymbol{x})dx. \tag{8.4}$$

On the other hand, the change of the entropy of the system is still determined by Eq. (2.18). Defining the entropy change in the environment ΔS_{env} by the thermodynamical relation (2.19), we infer that the total entropy production in the time interval $[0, t_f]$ is again given by the right hand side of Eq. (2.20):

$$\Delta S_{tot} = \Delta S_{sys} + \Delta S_{env} = \frac{1}{T}\int_0^{t_f} dt \int \big(\boldsymbol{v}\cdot M^{-1}\boldsymbol{v}\big)(t,\boldsymbol{x})\rho(t,\boldsymbol{x})dx, \tag{8.5}$$

see Refs. [15, 43] or [16] for the interpretation of ΔS_{tot} as a relative entropy of the processes with direct and time-reversed protocols along the lines proposed first in [39]. Equation (8.5) implies that the Second Law inequalities (2.21) and (2.22) still hold in the presence of non-conservative forces. Recall, that in the previous discussion, we minimized the right hand side of the above expression for ΔS_{tot} over all velocity fields with densities ρ evolving by the advection equation (2.5) between the fixed initial and final ones. Hence the bounds (6.3) and (6.4) providing a finite-time refinements of the Second Law still hold in the presence of non-conservative forces. They are saturated, nevertheless, by the dynamics with a conservative force that was constructed before: no protocol including non-conservative forces can lead to lower total entropy production or heat release than the optimal protocol with conservative forces.

9 Conclusions

We have established an exact lower bound (6.3) for the total entropy production in the overdamped Langevin dynamics with thermal noise that interpolates in a fixed time window between given statistical states with smooth positive probability densities. The bound, realizing

a refinement of the Second Law (2.21) of Stochastic Thermodynamics, is valid in the presence of conservative or non-conservative driving forces. It is inversely proportional to the length of the time window and to the temperature. The proportionality constant is given by the minimum of the quadratic cost function (4.10) over all deterministic maps transporting the initial probability distribution to the final one. The minimal entropy production occurs for the process driven by a conservative force with a time-dependent potential expressed by solutions of the inviscid Burgers equation related to the optimal Monge-Kantorovich mass transport and of the accompanying advection equation for densities. The refined Second Law (6.3) induced the optimal lower bounds (6.4) for the average heat release. The general theory was illustrated on the example of a model describing a mesoscopic particle manipulated by optical tweezers with a memory erasure dynamics of the type discussed in [17] as a toy model for Thermodynamics of Computation [8]. The system was recently studied experimentally [10] and we plan to use the outcome of the numerical analysis of our model to suggest an improvement of the experimental protocol in order to lower the average heat release in the process. Such an improved protocol will, in particular, implement over short time intervals the initial and final jumps of the optimal control potential.

The minimization of the average heat release, studied here, is closely related to the optimization of the average performed work, as was discussed in [48] and [3]. The results obtained here should have a simple extension to the case with limiting states given by probability measures without smooth densities. Such an extension would involve viscosity solutions of the inviscid Burgers equation admitting shocks. We have assumed in the analysis of the present paper that the configuration space of the system is $\mathbf{R}^d$. The effects of the nontrivial topology or geometry of the configuration space, will be discussed elsewhere. Applications of the optimal bounds on the entropy production or heat release to cyclic processes (e.g. to models of molecular motors and to optimization of their efficiency) is among natural directions of further research, see [20, 49] and the references therein. A more difficult problem requiring limiting arguments is an extension of the above results to the case of underdamped Langevin dynamics. A related discussion of work minimization in the Gaussian case may be found in [28]. Another step in that direction was taken recently in [4]. The question about the minimal entropy production in processes interpolating during a fixed time between fixed states makes sense for more general modelizations of non-equilibrium dynamics, e.g. for ones involving Markov processes with jumps and/or discrete state spaces [26, 27, 42, 50], see the recent work [46], for open quantum systems [12] (sometimes also described by jump processes), see the problem of work optimization in a model of quantum dot considered in [19], or for the ones involving thermostats [24]. It is certainly worth studying in such contexts as a more theoretical counterpart of Finite-Time Thermodynamics [14]. Other optimization problems of deterministic or stochastic nature related to fluctuation relations in non-equilibrium statistical mechanics may also be interesting [3]. The optimization techniques [5, 22] developed largely with an eye on other cost functions, seem to find this way new important applications.

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